FAST SOLVERS FOR MOVING MATERIAL INTERFACES: FINAL REPORT

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Abstract Our overall goal is to develop, implement and transfer accurate new numerical methods for solving moving boundary problems in materials science. We have three specific objectives:

- Combine semi-Lagrangian time stepping, accurate contouring and fast geometric algorithms to develop and implement accurate, efficient and general new methods for moving sharp interfaces.
- Develop a fast modular open source moving interface code for transfer to other researchers, labs, and industry.
- Build efficient, accurate and general integral solvers for coupled systems of partial differential equations (PDEs) modeling common material phenomena, and couple these solvers to our modular moving interface code.

We reached a milestone with respect to our first objective—an accurate, efficient and general moving interface method—with the semi-Lagrangian contouring method developed in References [16–20]. We are now finalizing portable C/C++ codes for fast adaptive accurate 2D contouring and general 2D and 3D moving interfaces, to attain our second objective. A 3D code has been developed, tested on viscoelastic flow [P0,P1,P2], and delivered for public availability on SourceForge. Our 2D code and a preliminary spectral solver based on Ewald summation has been implemented and thoroughly validated on 2D elastic membranes evolving in Stokes incompressible flow [P3]. Work is ongoing for a high-order linearly-implicit open-source 2D code for stiff interfaces. A fast and extremely robust elliptic solver with complex interfaces, based on a new immersed interface approach and a new Krylov-accelerated multigrid technique, has been developed, implemented and extensively validated on elliptic problems with high-contrast variable coefficients and complex interfaces [P4]. Finally, we are developing fast new elliptic PDE solvers, based on Ewald summation [P5], integral equations and a new geometric nonuniform FFT, to complete our third objective.

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Moving interfaces Our work on moving interface problems in materials science combines fast solvers such as boundary integral methods, deferred correction and Ewald summation with fast geometric algorithms and semi-Lagrangian implicit representations to build effective new numerical methods.

We developed an implicit boundary integral method for computing periodic dendrite formation in the symmetric model of unstable solidification [7] and fast algorithms for evaluating heat potentials [2] which speeded up our method by several orders of magnitude. In [6], we combined the boundary integral method of [7] with fast algorithms from [2,3,8] and the level set method of [4]: the level set method handled topological changes effectively while fast boundary integral techniques ensured accuracy and efficiency in the velocity evaluation. We developed and analyzed efficient and accurate new vortex methods for modeling convection in the melt [5,13,14,15], together with new error analyses [15] and quadrature rules [12] for general integral equations. In the interests of modeling arbitrarily complex material effects in the bulk, PDE solvers based on Ewald summation and analytic preconditioning were developed in [9,10,11]. Since then, we have focused on the development and implementation of highly effective new numerical methods for general moving interface problems and widely applicable related computations such as elliptic PDE solvers. We summarize three projects below: fast semi-Lagrangian contouring methods for general moving interfaces [16–20,P0–P2], Ewald summed boundary integral methods for Stokes flow with moving interfaces [P3], fast robust multigrid solvers for elliptic problems with complex interfaces [P4], and fast locally-corrected spectral methods for elliptic systems in periodic geometry [P5].

Moving interface problems A moving interface is a collection $\Gamma(t)$ of nonintersecting oriented closed curves (in $\mathbf{R^2}$) or surfaces (in $\mathbf{R^3}$). A sufficiently smooth moving interface has an outward unit normal vector N, a mean curvature C, and a normal velocity vector VN. A moving interface problem specifies VN as a functional of $\Gamma(t)$. Examples include passive transport $V = N \cdot F$ where $F(x,t)$ is given, geometric motion $V = p(\theta) - q(\theta)C$ where $\cos\theta = N \cdot \hat{x}$, Ostwald ripening $V = \left[\frac{\partial u}{\partial N}\right]$, where u solves the Laplace equation $\Delta u = 0$ off $\Gamma(t)$ and $u = C$ on $\Gamma(t)$, and models for crystal growth $V = \left[\frac{\partial u}{\partial N}\right]$, where u solves the heat equation $u_t = \Delta u$ off $\Gamma(t)$ with the geometric boundary condition $u = f(N, C, V)$ on $\Gamma(t)$.

A linearly-implicit approach Any moving interface problem can be reformulated as a PDE for a function φ whose zero set is $\Gamma(t)$. The normal, curvature and velocity are then

$$N = \frac{\nabla\varphi}{\|\nabla\varphi\|}, \qquad C = -\nabla \cdot N, \qquad VN = \frac{\varphi_t \nabla\varphi}{\|\nabla\varphi\|^2}.$$

Given an extension of VN off $\Gamma(t)$ to a globally defined function W, we can regard the VN formula as a PDE for φ:

$$\varphi_t - W \cdot \nabla\varphi = 0.$$

We solve this equation on an adaptive quadtree mesh to eliminate the cost of going up a dimension. Correct viscosity solutions are obtained by semi-Lagrangian time stepping with exact distancing and large time steps. A general problem-independent velocity extension makes our method modular and easy to apply.

Semi-Lagrangian methods The semi-Lagrangian "CIR" method [1] solves $\varphi_t - F(x,t) \cdot \nabla\varphi = 0$ by the following algorithm: at each evaluation point x at the new time level $t+k$, move x back with velocity $F(x,t_n)$ to $s = x + kF(x,t_n)$; interpolate $\varphi(x,t_n)$ to the point s; set $\varphi(x,t_{n+1})$ equal to the interpolated value. Our second-order time stepping scheme couples a CIR predictor with a trapezoidal corrector using the velocity evaluated from the CIR approximation. It combines the unconditional stability of CIR with the dramatically reduced dissipation of the trapezoidal rule. Interpolation error is eliminated by exact distance finding in a dynamic quadtree data structure. The tree mesh is refined with a functional approach: given a signed distance function $\varphi(x,t_n)$, we build a tree at time $t_{n+1} = t_n + k$ by recursive evaluation of $\varphi(x,t_{n+1}) = \varphi(s,t_n)$ at projected points $s = x + kF(x,t_n)$.

Our semi-Lagrangian method for moving interfaces [19] combines efficient exact quadtree-based redistancing, stable second-order semi-Lagrangian time stepping, a modular problem-independent velocity extension, and exact φ interpolation in the CIR scheme. The velocity extension technique evaluates the nearest-point extension on a distance tree, builds a continuous interpolant, and satisfies a maximum principle. Our method resolves and moves complex interfaces at optimal cost with time steps unconstrained by numerical stability. It is a "black-box" method for moving interfaces, which accepts the interface and its velocity at time t and returns the evolved interface one time step later. Such methods simplify moving interfaces, because the numerics are independent of the physical problem driving the interfacial motion. Numerical results show that the method converges to correct viscosity solutions even for difficult moving interface problems involving merging, faceting, transport, nonlocality and anisotropic curvature-dependent geometry.

A fast semi-Lagrangian contouring method [20] General moving interface problems are solved in [20] by a new approach: extract the moving interface from an explicit semi–Lagrangian advection formula with efficient geometric algorithms and fast accurate contouring techniques. A modular adaptive implementation with fast new geometry modules computes highly accurate solutions to moving interface problems involving merging, anisotropy, faceting, curvature, dynamic topology and nonlocal interactions of PDE type. Exact geometric algorithms are tuned for speed; velocity evaluation and time stepping are efficiently decoupled from interface resolution; fast new contouring techniques dramatically increase overall accuracy. An efficient adaptive framework combines the high resolution of front tracking with the topological robustness of implicit representations.

Accurate contouring The general problem of finding a smooth geometrically constrained approximate zero set of a function which can be evaluated at arbitrary points

occurs frequently in computational science and requires a robust general contouring package. An ideal contouring package would accept function values (and derivatives if available) at arbitrary points and produce a piecewise-smooth approximation to the zero set with corners where necessary. Geometric constraints such as bounds on curvature away from corners are vital in applications such as computer-controlled machining, and pose a major complication for existing public-domain contouring software. The PI, with a graduate student, is finalizing new open-source C/C++ packages for constrained piecewise-smooth contouring of scattered data in two and three dimensions.

Ostwald ripening We are building fast nonlocal velocity evaluation modules for several standard moving interface problems of materials science. The simplest example is Ostwald ripening, which models the growth of larger solid drops by evaporation from smaller drops with total solid volume conserved. The velocity V is the normal derivative $\left[\frac{\partial u}{\partial N}\right]$ of the function u which is harmonic off $\Gamma(t)$ and equal to the curvature on $\Gamma(t)$. We evaluate this nonlocal velocity by solving the integral equation of classical potential theory and applying the Dirichlet to Neumann operator. The solution u is a double layer potential

$$D\mu(x) = \int_\Gamma \frac{\partial K(x,y)}{\partial N(y)} \mu(y) dy$$

of an unknown density μ on $\Gamma = \Gamma(t)$, with $K(x,y) = \frac{1}{2\pi} \log \|x - y\|$ the free-space Green function for the two-dimensional Laplace equation. The density μ solves the integral equation

$$\frac{1}{2}\mu(x) + \int_\Gamma \frac{\partial K(x,y)}{\partial N(y)} \mu(y) dy = C(x), \qquad x \in \Gamma.$$

Once μ is found, it is convenient to view the harmonic function u as the real part of an analytic function U. The Cauchy-Riemann equations then yield V as the tangential derivative of the imaginary part of U, which is easier to compute than the normal derivative of the real part u. Discretization of this formulation is highly accurate if the interface is represented by equidistant points in arclength. Detailed resolution of the interface requires many points, so fast algorithms such as the fast multipole method play an important role.

3D viscoelastic flow with interfaces The semi-Lagrangian method has been implemented in 3D and coupled with a viscoelastic fluid simulator to produce complex and realistic fluid simulations [P0,P1,P2]. A particularly useful feature of the semi-Lagrangian approach is the convenience of tracking local features such as textures on the surface.

Stokes flow with interfaces [P3] Many biological moving interface problems (blood flow, cell movement, atherosclerosis) involve slow viscous flows satisfying the

incompressible Stokes equations

$$-\nu\Delta u + \nabla p = F, \qquad \nabla \cdot u = 0.$$

Elastic interfaces produce singular forces $F = f\delta_\Gamma$ where δ_Γ is a measure on the interface Γ. We have developed a fast solver for such problems by combining semi-Lagrangian interface evolution with a fast new Ewald summation scheme for the Stokes equations. The semi-Lagrangian transport of interface densities allows a straightforward computation of stretching energy, while the new fast summation technique unifies several well-known local correction techniques for singular integral operators. Our fast summation technique is particularly effective for Stokes problems with discontinuous data such as elastic membrane problems, where standard methods encounter great difficulty. Circularizing and oscillating interfaces under Stokes flow are computed accurately to one part per thousand.

Elliptic solvers with complex interfaces [P4] A new piecewise-polynomial interface method (PIM) for discretizing elliptic problems with complex interfaces between high-contrast materials is derived, analyzed and tested. A Krylov-accelerated interface multigrid approach (IMG) solves the discretization efficiently. Stability and convergence are proved in one dimension, while an extensive array of numerical experiments with complex interfaces and large coefficient transitions demonstrate the accuracy, efficiency and robustness of the method in two dimensions.

Ewald summation for elliptic systems [P5] Our Stokes solver generalizes to solve general overdetermined constant-coefficient elliptic systems

$$A_j u_{,j} + A_0 u = f$$

subject to periodic boundary conditions. Thus every constant-coefficient linear elliptic problem can be solved with a single automatic code, eliminating the necessity for many specialized codes. Our approach yields high-order accuracy even for solutions with limited smoothness, and combines with a distributional approach to arbitrary domains to yield solvers promising arbitrary order accuracy and almost optimal efficiency.

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Interactions/Transitions The PI presented results from this research in seminars and colloquia at American Institute of Mathematics, Brown University, Courant Institute, Duke University, Fields Institute for the Mathematical Sciences, Free University of Berlin, Georgia Tech, Hong Kong University of Science and Technology, INRIA Rocquencourt, Michigan State University, Naval Postgraduate School, North Carolina State University, Statistical and Applied Mathematics Institute, Stanford University, Technical University of Berlin, Technical University of Munich, Texas A&M University, Universite Joseph Fourier Grenoble, University of California at Berkeley, University of California at Davis, University of California at Santa Cruz, University of North Carolina at Charlotte, University of Texas at Austin, University of Pennsylvania, 2nd International Meeting on Scientific Computing and Partial Differential Equations, ICIAM 2007, and SIAM 2005 Annual Meeting,

An efficient and accurate 2D contouring code is nearing completion, and will soon be freely available from the PI's website. Several fast transform codes and a fast 2D solver for parabolic partial differential systems are already available, and deferred correction/multigrid/boundary integral codes for two-point and elliptic boundary value problems are in progress. The 3D surface tracking method described in [P0,P1,P2] has been implemented as part of the Berkeley Fluid Animation and Simulation Toolkit (BFAST), which has been open source released and is available on SourceForge.

Publications [P0] A. W. Bargteil, J. F. O'Brien, T. G. Goktekin, and J. Strain, 2005, "A semi-Lagrangian contouring method for fluid simulation."
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